

# **New alkoxyphenyl substituted benzo[1,2-b:4,5-b'] dithiophene-based polymers: synthesis and application in solar cells**

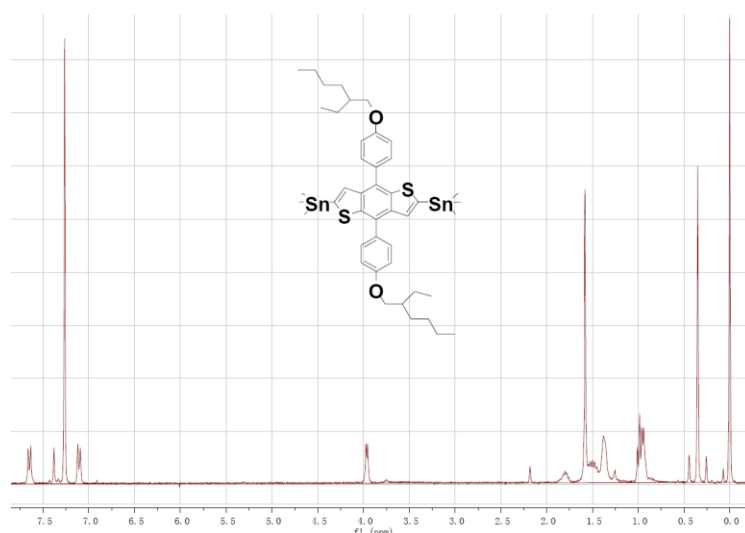
**Jun Yuan,<sup>‡a</sup> Lu Xiao,<sup>‡a</sup> Bo Liu,<sup>‡ab</sup> Yongfang Li,<sup>c</sup> Yuehui He,<sup>b</sup> Chunyue Pan,<sup>a</sup> Yingping Zou<sup>\*a,d</sup>**

<sup>a</sup> *College of Chemistry and Chemical Engineering, Central South University, Changsha 410083, China E-mail: [yingpingzou@csu.edu.cn](mailto:yingpingzou@csu.edu.cn)(Y.Zou)*

<sup>b</sup> *State key Laboratory for Powder Metallurgy, Central South University, Changsha 410083, China*

<sup>c</sup> *Beijing National Laboratory for Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China*

<sup>d</sup> *Key Laboratory of Resources Chemistry of Nonferrous Metals (Central South University), Ministry of Education, Changsha, Hunan 410083, China*



**Fig.S1**  $^1\text{H}$  NMR spectroscopy of the BDTPO monomer

**Table S1:** Optical and Electrochemical Properties of the Synthesized Conjugated Copolymers

Polymers	Absorption spectra				Cyclic voltammetry		
	Sol <sup>a</sup>		Film <sup>b</sup>		<i>p</i> -doping	<i>n</i> -doping	$E_g^{EC}$ (eV)
	$\lambda_{\max}$ (nm)	$\lambda_{\max}$ (nm)	$\lambda_{\text{onset}}$ (nm)	$E_g^{opt}$ <sup>c</sup> (eV)	$E_{\text{on}}^{ox}$ /HOMO <sup>d</sup> (V)/(eV)	$E_{\text{on}}^{red}$ /LUMO <sup>d</sup> (V)/(eV)	
<b>PBDTPO-DTBO</b>	575	567	749	1.65	1.16 /-5.56	-0.72 /-3.68	1.88
<b>PBDTPO-DTBT</b>	540	556	765	1.62	1.06/-5.46	-0.74/-3.66	1.80

a. Measured in chloroform solution. b. Cast from chloroform solution. c. Bandgap estimated from the onset wavelength of the optical absorption. d. HOMO =  $-e (E_{\text{on}}^{ox} + 4.4)$  (eV); LUMO =  $-e (E_{\text{on}}^{red} + 4.4)$  (eV) using (eV) using Ag/AgCl as the reference electrode.

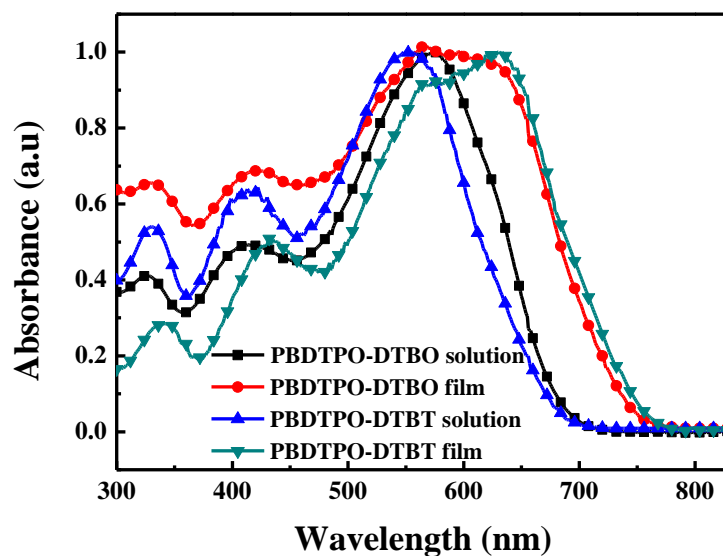


Fig. S2 UV-Vis absorption spectra of PBDTPO-DTBO and PBDTPO-DTBT in  $\text{CHCl}_3$  and films

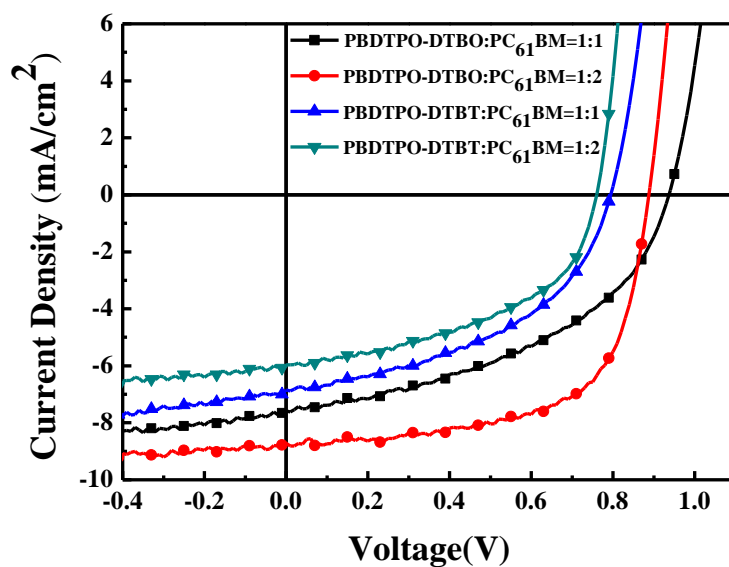
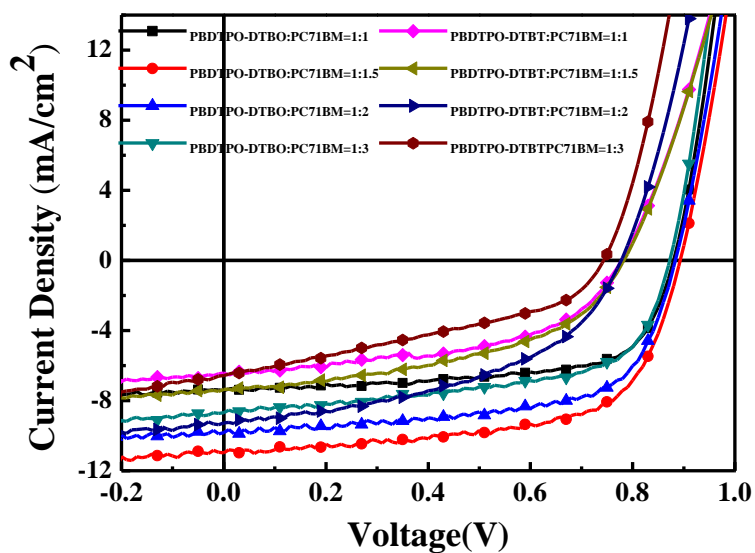


Fig. S3  $J-V$  curves of the PSCs based on PBDTPO-DTBO and PBDTPO-DTBT:  $\text{PC}_{61}\text{BM}$ , under illumination of AM 1.5,  $100 \text{ mW}/\text{cm}^2$ .

**Table S2** Photovoltaic Data of Polymer Solar Cells Based on PBDTPO-DTBO and PBDTPO-DTBT Blended with PC<sub>61</sub>BM

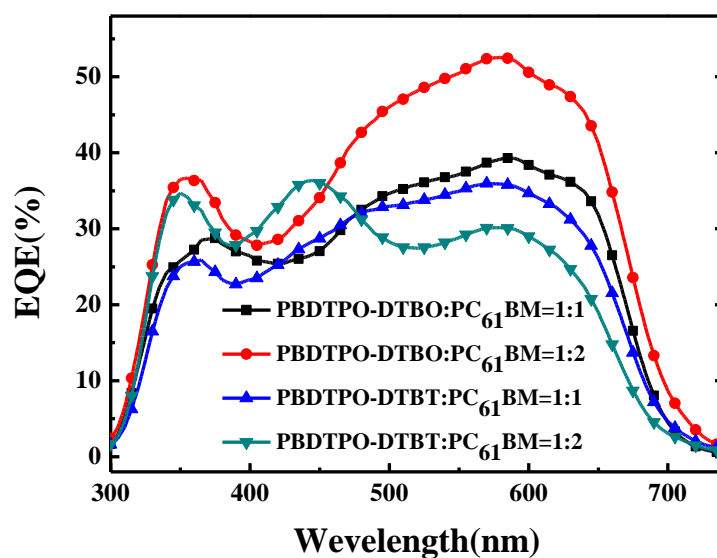
Active layer	V <sub>oc</sub> (V)	J <sub>sc</sub> (mAcm <sup>-2</sup> )	FF (%)	PCE (%)
PBDTPO-DTBO:PC <sub>61</sub> BM=1:1	0.94	7.6	45	3.2
PBDTPO-DTBO:PC <sub>61</sub> BM=1:2	0.89	8.7	64	5.0
PBDTPO-DTBT:PC <sub>61</sub> BM=1:1	0.79	6.9	47	2.6
PBDTPO-DTBT:PC <sub>61</sub> BM=1:2	0.76	6.0	48	2.2



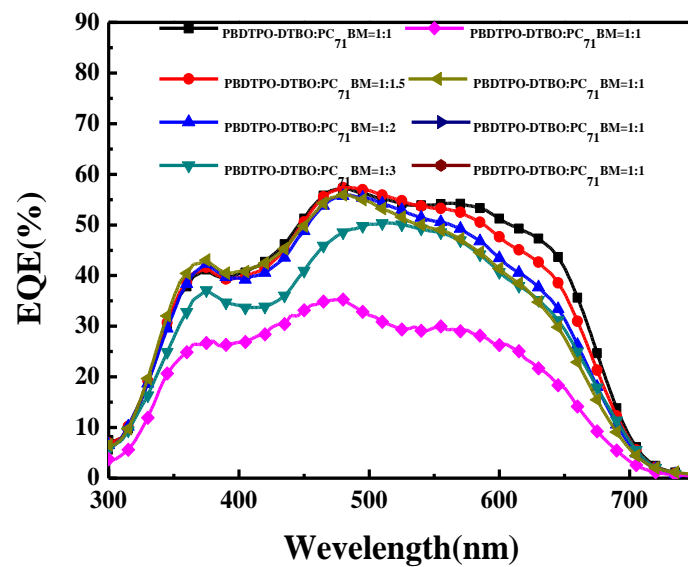
**Fig.S4** *J-V* curves of the PSCs based on polymers: PC<sub>71</sub>BM, under illumination of AM 1.5, 100 mW/cm<sup>2</sup>.

**Table S3:** Photovoltaic Data of the Polymer Solar Cells Based on PBDTPO-DTBO and PBDTPO-DTBT Blended with PC<sub>71</sub>BM

Active layer	V <sub>oc</sub> (V)	J <sub>sc</sub> (mAcm <sup>-2</sup> )	FF (%)	PCE (%)
PBDTPO-DTBO:PC <sub>71</sub> BM=1:1	0.90	9.5	56	4.8
PBDTPO-DTBO:PC <sub>71</sub> BM=1:1.5	0.89	11	64	6.2
PBDTPO-DTBO:PC <sub>71</sub> BM=1:2	0.88	9.8	65	5.6
PBDTPO-DTBO:PC <sub>71</sub> BM=1:3	0.87	8.7	59	4.5
PBDTPO-DTBT:PC <sub>71</sub> BM=1:1	0.78	6.4	51	2.6
PBDTPO-DTBT:PC <sub>71</sub> BM=1:1.5	0.78	7.4	48	2.8
PBDTPO-DTBT:PC <sub>71</sub> BM=1:2	0.78	9.3	47	3.4
PBDTPO-DTBT:PC <sub>71</sub> BM=1:3	0.74	6.6	38	1.8



**Fig.S5** EQE spectra of PSCs based on PBDTPO-DTBO and PBDTPO-DTBT: PC<sub>61</sub>BM (1:1 and 1:2, w/w).



**Fig.S6** EQE spectra of PSCs based on PBDTPO-DTBO and PBDTPO-DTBT: PC<sub>71</sub>BM (1:1, 1:1.5, 1:2, and 1:3 w/w).